Procedure for Separating Main ChemFinder (.cfw) file into Tested Form SDF (Main) and Defined Organic Parent SDF (DOP) using ChemOffice 2000 ChemFinder (ver. 7.0) (*13Oct03*)

Main ChemFolder file used in DSSTox development has 2 structures fields containing the tested form structure and defined organic parent structures.

Creation of Main SDF file for creating TF and DOP SDF files:

1. Open **ChemFinder**.
2. Select **Open** from the file menu.
3. Select the Main ChemFinder file (containing 2 structures and full complement of TF and DOP fields)
4. Check to see that all fields are present, and that all field names are in final form.
5. Follow process for reordering fields as laid out in *"Procedure for ExportingChemFinderFile_to_FinalSDF"*, use same field names.

Creation of Main TF SDF file:

1. Save Main ChemFolder file to new ChemFolder file named "NAMEID_v#x_###_ddmmmyy_TF_export".
2. Create new subfolder NAMEID_TF_ddmmmyy.
3. Click on Arrow button on left menu bar; select and delete: Structure1, Formula1, MolWeight1, CAS DOP, SMILES DOP, and StructureShown DOP fields. Save.
4. Delete Mol_ID field. If DevelopmentNote field exists, delete this also.
5. **File → Export → SDFile**, saving SDF file to new subfolder named NAMEID_TF_ddmmmyy.
6. Follow procedure for *"Cleaning and Finalizing SDF"*.
7. Import clean SDF file into ChemFinder and ChemFolder to check fields, content and field ordering.

Creation of Defined Organic Parent (DOP) SDF file:

1. Save Main ChemFolder file to new ChemFolder file named "NAMEID_v#x_###_ddmmmyy_DOP_export".
2. Select and export only "defined organic" records to SDF:
   a. From Main ChemFolder file, select **Enter Query** from the **Find** Menu or PRESS **Ctrl+ f**.
   b. Enter ***defined organic*** in the field labeled **substance type** and press **Enter**
   c. Without deleting any fields, select **Export → SDFile** from File Menu.
   d. **Save As** the standard name with the addition of the **_DOP** extension into new subfolder named NAMEID_DOP_ddmmmyy.
2. Import SDF in Microsoft Excel for editing to DOP format:
   a. Open Microsoft Excel, select **Add-in…** from the **Tools** Menu.
   b. Check box associated with ChemDraw for Excel (ChemFinder Version 7.0 2002 or later) or ChemFinder for Excel (ChemFinder Version 6.0 2001 or earlier).
   c. Select **OK** (a new toolbar and menu will be displayed titled ChemDraw or ChemFinder respectively.

d. Select **Convert/Update Worksheet** from the **ChemDraw/ChemFinder** menu.

e. Select **Import Table** from the **ChemDraw/ChemFinder** menu.

f. Select the SDF file for which the DOP file is to be created.

3. Edit SDF file in Microsoft Excel to DOP format:

   a. Select the Column labeled "SMILES_DOP", and select **Copy** from the **Edit** menu.

   b. Select **Column A**, and select **Paste** from the **Edit** menu to paste contents of "SMILES_DOP" into Structure Field.

   c. Replace **Column A** header (cell A1) with the title "STRUCTURE".

   d. Select Column A again.

   e. Select **Convert SMILES to Molecule** from the **ChemDraw/ChemFinder** menu.

   f. All values but 1 (title header) should be converted.

   g. For values not converted:

      i. Copy the structure from the main ChemFinder file which is still open for the corresponding structure/record

      ii. Double click on the SMILES code in column A

      iii. ChemDraw will open. Press **Ctrl+V** to paste the structure.

      iv. Press **Ctrl+W** to return **to ChemDraw/ChemFinder for Excel**.

      v. Continue this process for values not converted

   h. Edit Column titled "DSSTox_FileName" to reflect new filename with _DOP extension, using global find/replace of NAMEID_v#x_ddmmmyy with NAMEID_DOP_v#x_ddmmmyy

   i. Delete column "StructureShown" and rename column "StructureShown_DOP" to "StructureShown".

   j. Insert new column before CAS column and paste contents of CAS_DOP into this new column; select and delete old CAS_DOP column.

   k. Rename CAS column to CAS_TestedForm, and CAS_DOP to CAS.

   l. Insert new column before SMILES column and paste contents of SMILES_DOP into this new column; select and delete old SMILES_DOP column.

   m. Rename SMILES column to SMILES_TestedForm, and SMILES_DOP to SMILES.

   n. If DevelopmentNote column exists, delete this also.

2. Select Export Table from the **ChemDraw/ChemFinder** menu.

3. Save as the standard file name with the _DOP extension into the folder NAMEID_DOP_ddmmmyy.

4. Write over the existing file of the same name.

5. Follow procedure for *"Cleaning and Finalizing SDF"* .

6. Import new DOP SDF file into ChemFinder and ChemFolder to check fields, content and field ordering.